Benzoic acid, 4-methoxy-
100-09-4 | DTXSID4059205

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.62e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

Image not found
(Cyclopentyloxy)acetic acid
Measured: 1.42e-01
Predicted: 1.96e-01

Image not found
Phenylalanine
Measured: 1.34e-01
Predicted: 3.30e-01

Image not found
Phenylalanine
Measured: 1.34e-01
Predicted: 3.30e-01

Image not found
D-Phenylalanine
Measured: 1.34e-01
Predicted: 3.30e-01

Image not found
Penicillic acid
Measured: 1.18e-01
Predicted: 1.39e-01

Image not found
6-Aminocaproic acid
Measured: 3.85
Predicted: 4.69

Image not found
2-Propenoic acid, 3-(2-furanyl)-
Measured: 1.45e-02
Predicted: 3.48e-01